Sebacic acid, 2-acetylphenyl isohexyl ester

Inchi: InChI=1S/C24H36O5/c1-19(2)13-12-18-28-23(26)16-8-6-4-5-7-9-17-24(27)29-22-15-11-1

InchiKey: DMWGFPIKOKSOGV-UHFFFAOYSA-N

Formula: C24H36O5

SMILES: CC(=O)c1ccccc1OC(=O)CCCCCCCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-345.22	kJ/mol	Joback Method
hf	-921.09	kJ/mol	Joback Method
hfus	55.22	kJ/mol	Joback Method
hvap	96.63	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.895		Crippen Method
mcvol	341.710	ml/mol	McGowan Method
pc	1079.93	kPa	Joback Method
rinpol	2997.00		NIST Webbook
tb	986.19	K	Joback Method
tc	1207.44	K	Joback Method
tf	578.43	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.74	J/mol×K	986.19	Joback Method
cpg	1149.75	J/mol×K	1023.07	Joback Method
cpg	1163.27	J/mol×K	1059.94	Joback Method
cpg	1175.34	J/mol×K	1096.82	Joback Method
cpg	1186.01	J/mol×K	1133.69	Joback Method
cpg	1195.30	J/mol×K	1170.57	Joback Method
cpg	1203.27	J/mol×K	1207.44	Joback Method
dvisc	0.0003398	Pa×s	578.43	Joback Method
dvisc	0.0001775	Pa×s	646.39	Joback Method

dvisc	0.0001049	Pa×s	714.35	Joback Method
dvisc	0.0000679	Pa×s	782.31	Joback Method
dvisc	0.0000472	Pa×s	850.27	Joback Method
dvisc	0.0000346	Pa×s	918.23	Joback Method
dvisc	0.0000264	Pa×s	986.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume